Supporting information for:

Proton-coupled hopping in Ru-modified *P. aeruginosa* azurin

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Contents:

1. Mass spec characterization of Ru-labeled proteins

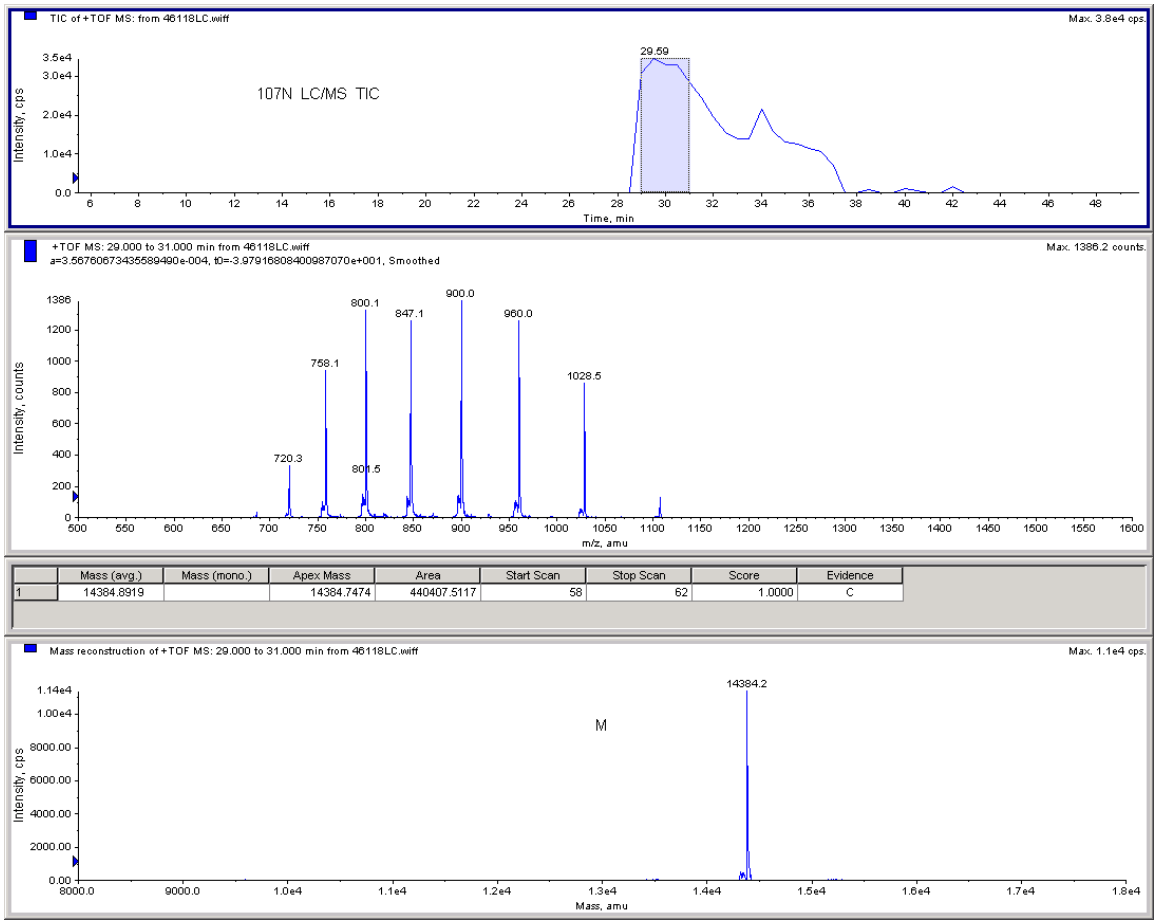
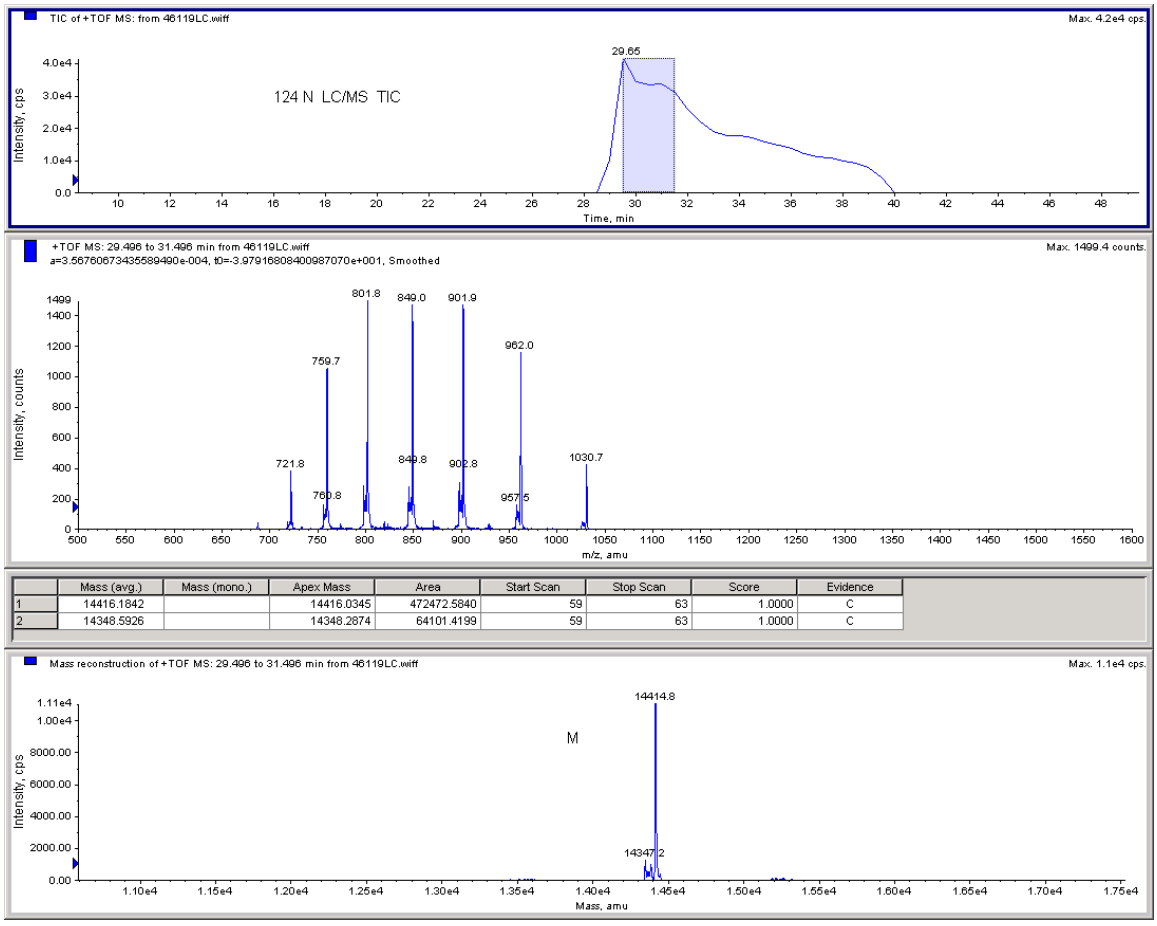


Figure S1. Liquid chromatography-mass spec for RuH107YOH109 azurin. Expected mass: 14388 Da; observed mass: 14384 Da.



	Mass (avg.)	Mass (mono.)	Apex Mass	Area	Start Scan	Stop Scan	Score	Evidence
1	14416.1842		14416.0345	472472.5840	59	63	1.0000	C
2	14348.5926		14348.2874	64101.4199	59	63	1.0000	C

Figure S2. Liquid chromatography-mass spec for RuH124YOH122 azurin. Expected mass: 14418 Da; observed mass: 14415 Da. The MS for RuH126YOH122 is identical, as the proteins have the same expected masses.

2. pK_a of YOH107 and YOH124

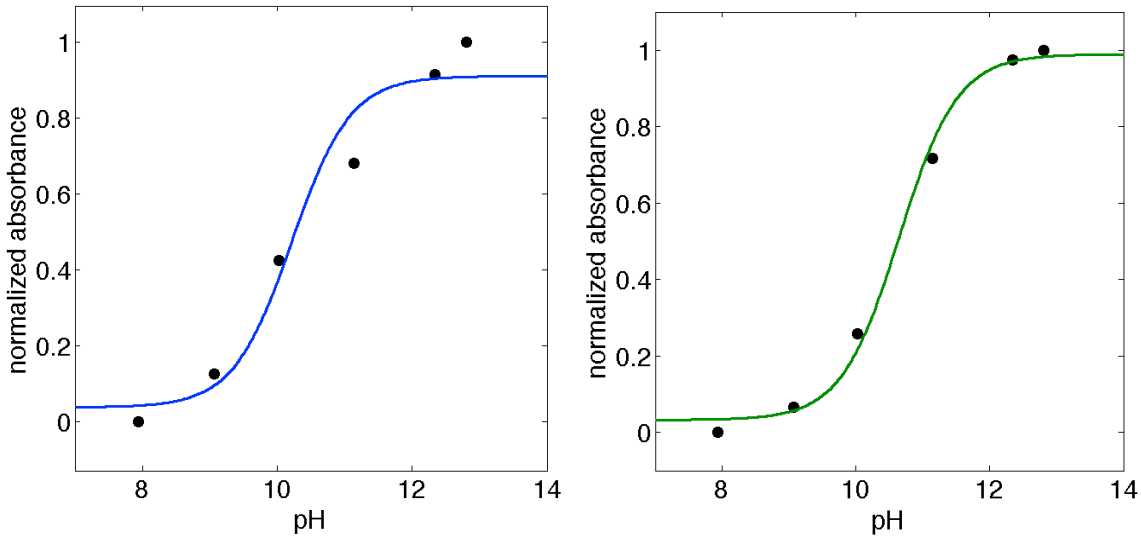


Figure S3. Titration data for H107YOH109Cu^{II} (left) and H122YOH124Cu^{II} (right) azurins. Data were collected in 250 mM sodium borate + 100 mM NaCl at 293 K. The fits (see main text) give pK_a(YOH109) = 10.2 ± 0.2 and pK_a(YOH122) = 10.6 ± 0.1.

3. Buffer concentration dependence kinetics traces.

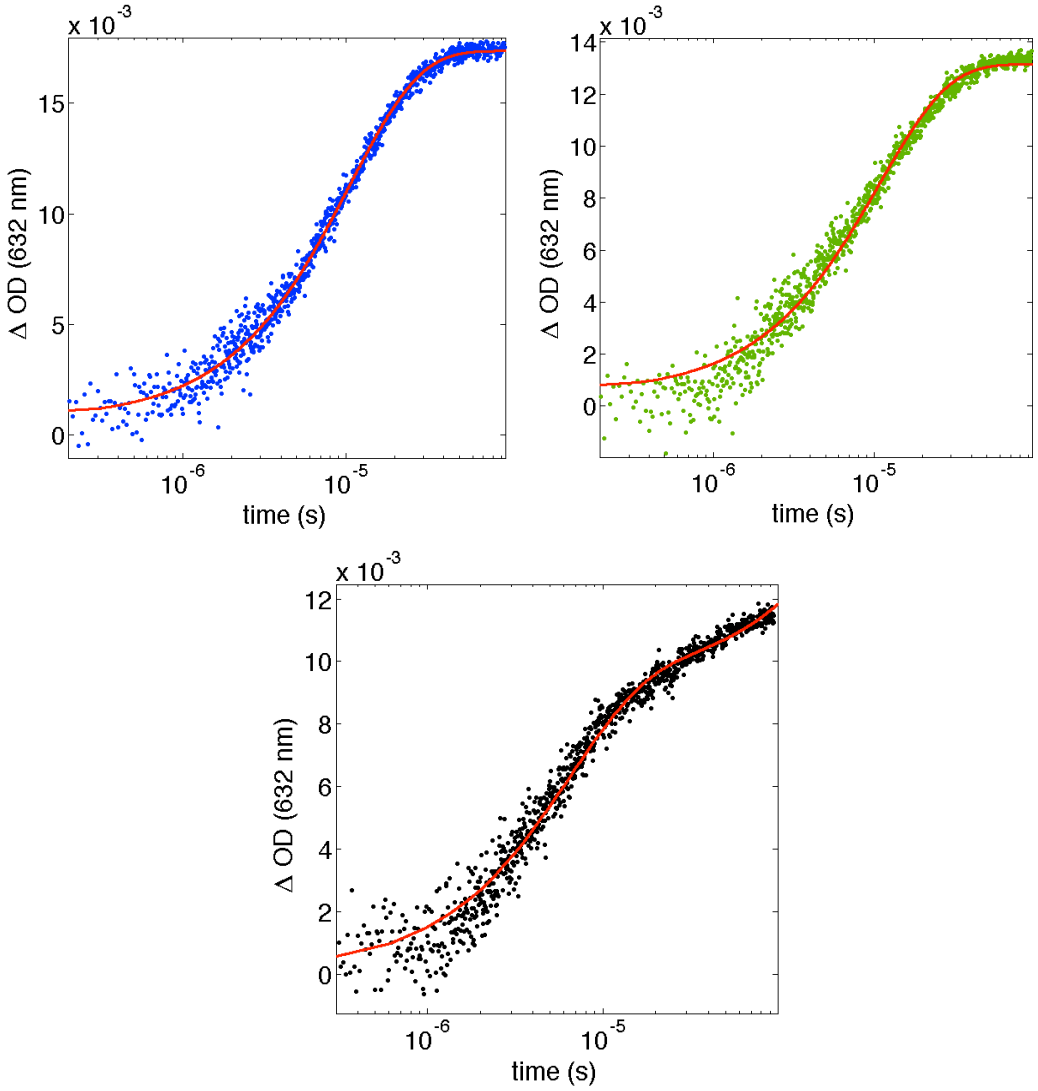


Figure S4. Kinetics traces for RuH124YOH122 Cu^{I} oxidation in imidazole buffer at pH 8. (A) 250 mM (as in the main text). (B) 100 mM. (C) 10 mM with a biexponential fit. $k_1 = 1.6 \times 10^5$ and $k_2 = 2.5 \times 10^3$.

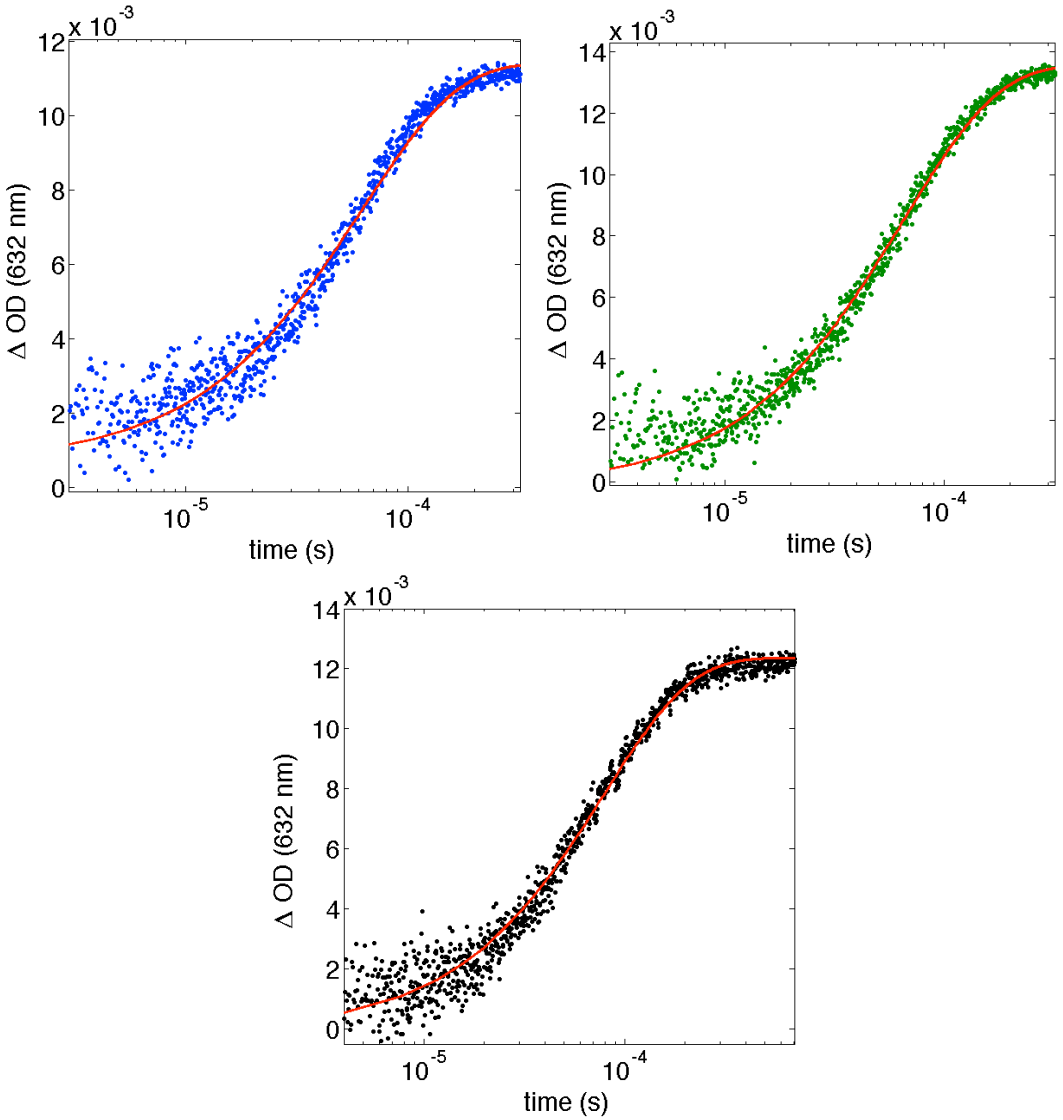


Figure S5. Kinetics traces for RuH107YOH109 Cu^{I} oxidation in imidazole buffer at pH 8. (A) 250 mM (as in the main text). (B) 100 mM. (C) 10 mM.

4. Kinetics traces in different buffers

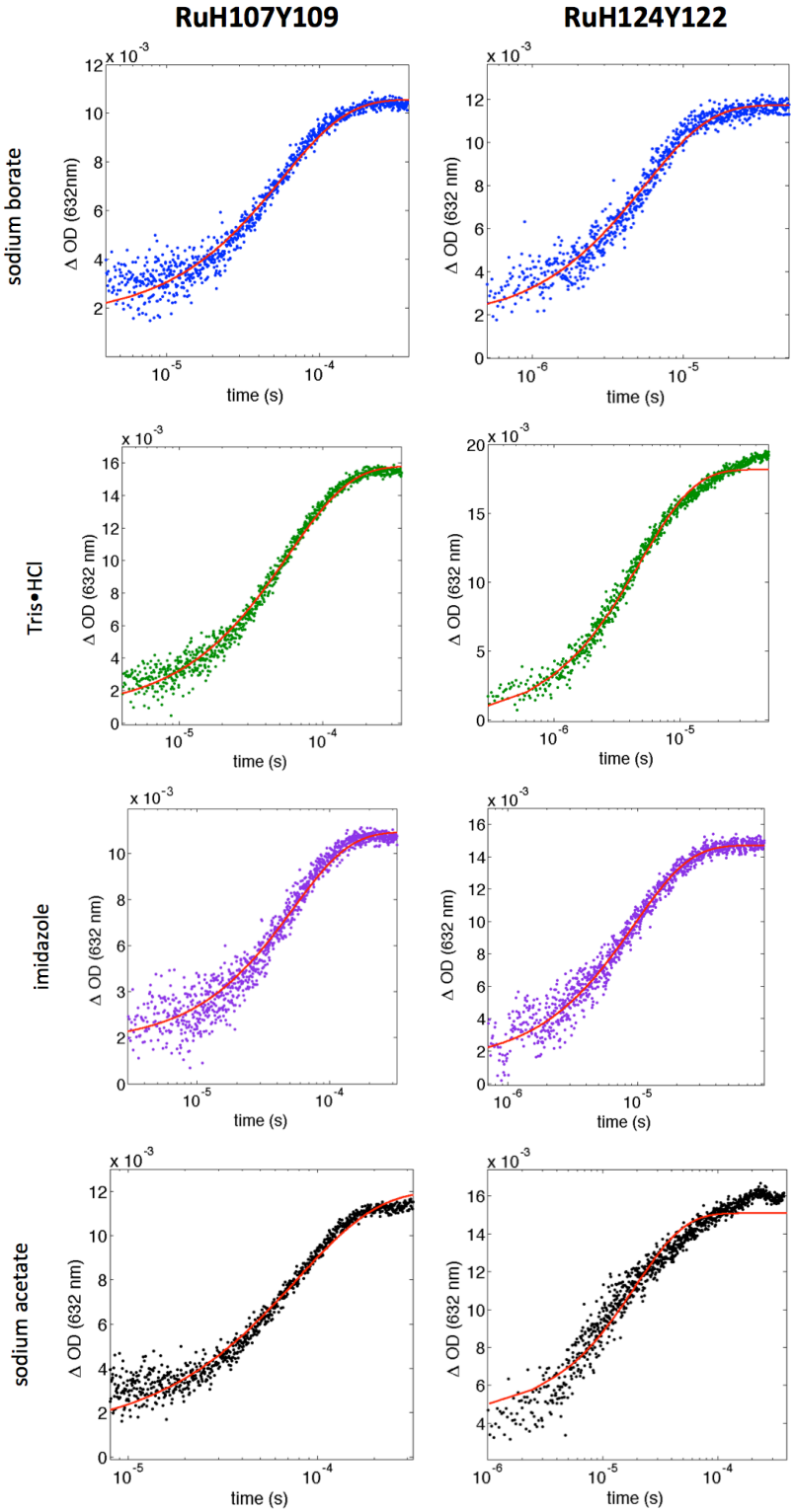


Figure S6. Kinetics traces for Cu^{I} oxidation in different buffers (all 250 mM, pH 8). The left column shows data for RuH107Y109 azurin and the right column shows the data for RuH124Y122 azurin. Buffer pK_as are: 9.14 (borate); 8.07 (Tris); 7.05 (imidazole); 4.76 (acetate).